FE Modeling of Surfaces with Realistic 3D Roughness: Roughness Effects in Optics of Plasmonic Nanoantennas

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Abstract: COMSOL Multiphysics has been widely used to model the near and far-field electromagnetics (specifically, transmission and reflection spectra) of gold and silver nanoantenna arrays [1,2,3]. However, previous models have used ideal (smooth) geometries, and degraded experimental performance due to surface roughness, interior defects, and other effects is taken into account through a single value, a material 'loss factor'. 1-D roughness has been introduced into simulations for single-period plasmonic metamagnetics[4], however there, the mesh was regenerated for each statistical realization of the roughened boundary. Here we use a moving 3D mesh, thus preserving the DOF number and simply morphing the structure of the mesh to accommodate the moving boundary.

Keywords: electromagnetics, resonance, nanoantennas, roughness

1. Introduction

Nanoantenna models are typically meshed using a 'normal' quality free-mesh. In this study we use a more complicated meshing procedure to simulate the effects of a roughened structure.

This study, however, first applies a moving mesh model in order to map a statistically defined roughness onto the surface of the antennas in a user-controlled manner. In our case specifically, the mesh on the flat surfaces of the antennas are displaced using 48 2D-Gaussian bumps with a defined amplitude of either positive (bump out) or negative (bump in) values, and a defined full-width half-max. There are an equal number of 'in' and 'out' bumps, although they are spread randomly over the surface. A moving mesh solver is initially used, leading to a model with roughened surfaces. Both the original 'smooth' mesh, and the displaced 'rough' mesh are saved and loaded into a separate electromagnetics model. Rearranging the profiles over the surface of the antenna is done simply by indexing the array of bump amplitudes or 'rotating' the bumps, leading to different roughness profiles, but with the same statistical qualities. The mapped mesh is used on the antenna surface so that when the bumps are rearranged to different locations each bump will maintain the same profile regardless of its 'rotated' or rearranged position. A free mesh, which is nonuniform over the surface, would cause a single bump with a constant definition to appear different depending on the mesh where it is placed. This methodology allows us to properly model the effect of surface roughness on nanoantenna performance.

2. Use of COMSOL multiphysics

A typical smooth nanoantenna array unit cell is shown in Figure 1, where the surface of the antennas uses a mapped mesh. The grid size of the mapped mesh is defined by setting a maximum element size for each edge. Free meshes are used for the air and glass regions.

Examples of the resulting roughened nanoantennas are shown in Figure 2 for two different roughness arrangements. In the example shown here, nanoantennas were modeled with a unit cell size of 400 nm by 400 nm. Their x,y dimensions are 108 nm by 102 nm respectively with a thickness of 36nm. The gap between the two nanoantennas is 28 nm. The antennas are modeled using a Drude – Lorentz model[2] for gold with a loss factor of 1.3. To understand the effect of roughness on the electromagnetic response of these nanoantennas, roughness profiles with amplitudes of both ±5 nm and ±10 nm, and a full-width half-max of 20nm, are compared to the smooth antenna model.

Electromagnetics are then applied using TE and TM mode plane waves through the RF module, with boundary conditions and a primary (P) E-field polarization as shown in Figure 1, and a secondary polarization (S) with the field rotated 90 degrees (and an appropriate switching of boundary conditions), and then solved using harmonic propagation analysis. The

electromagnetics model consist of four multiphysics models, two for each polarization: one with all materials set to air as a reference, and one with the proper nanoantenna materials. All the models use the same geometry and mesh. The reference field is used to calculate transmission and reflection of the nanoantenna models.
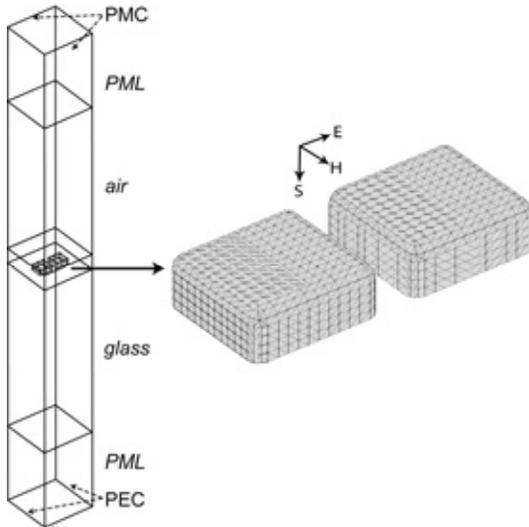
Figure 1: Schematic of a nanoantenna unit cell
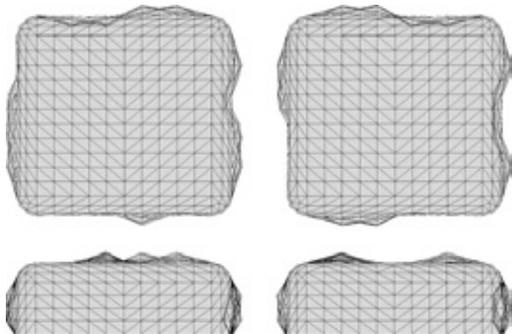
**Figure 2:** Example nanoantenna roughness iteration 1.
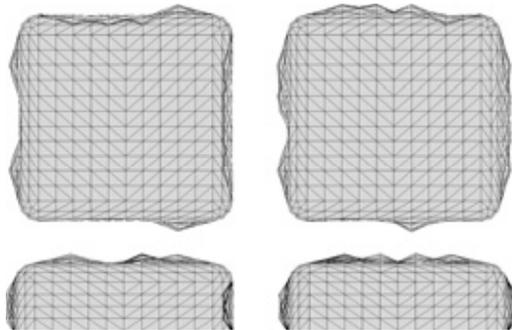
Figure 3: Example nanoantenna roughness iteration 2.

The final mesh in our example contains about 48 thousand elements, giving each of the four electromagnetics models 943 thousand DOF. These simulations were ran on a single cluster node with 8 Quad-Core Intel E5410 2.33GHz processors and 16GB of memory. Solutions were found for 9 wavelengths in Comsol version 3.5a with Matlab in script mode. Solution times varied, but averaged around 9 hours for each of the four multiphysics models.

3. Results

By comparing the far-field transmission and reflection spectra for the smooth mesh model (an ideal nanoantenna) to the spectra for various arrangements of roughness (a rough nanoantenna), we may determine the effects of surface roughness onto the electromagnetic performance of the nanoantennas. Specifically, we may isolate the effect of geometric surface roughness from other effects to due internal material properties on the plasmonic performance of the nanoantennas.

In Figures 4 and 5 we see the results for several iterations (roughness arrangements) of each roughness profile (5nm and 10nm bump amplitude). These multiple iterations were averaged to represent the results from an array of many nanoantennas, as is present in the actual sample. The resulting averaged spectra are shown in Figures 6 and 7. By comparing the smooth antenna model with the results from each of the rough models, we see that surface roughness does not significantly increase the magnitude of the resonant absorption, but instead produces a shift in the resonance wavelength. This might be due to the roughness inducing a variation in the width of the gap, which will affect the resonant wavelength. It is important to note that while the loss-factor modeling parameter, a single value typically incorporating roughness along with many other physical material properties and discussed elsewhere[3,4], usually results in a strong decrease in the strength of the resonance, roughness alone does not significantly reduce the resonance, but does result in a shift of wavelength. This means that the effects of surface roughness, which are typically incorporated into loss-factor, may be distinguished separately if the model properly accounts for surface roughness, as has been done here.
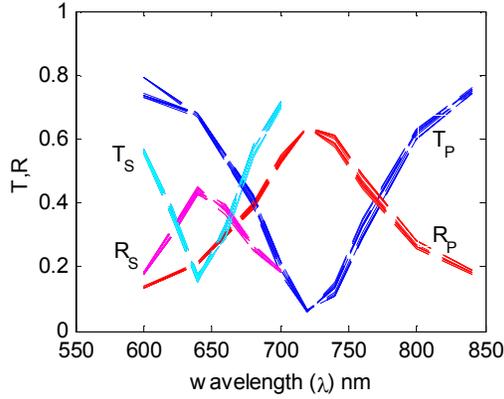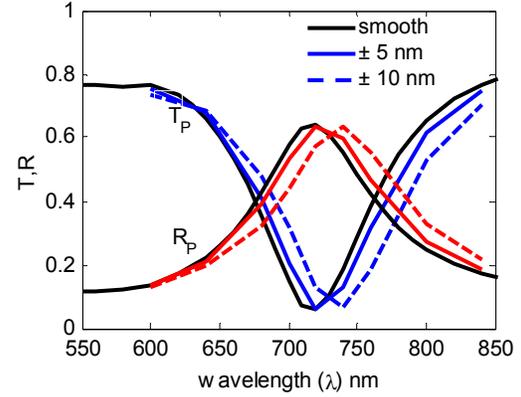
Figure 4: Transmission and Reflection spectra for the primary (P) and secondary (S) polarizations for various 5nm roughness iterations.
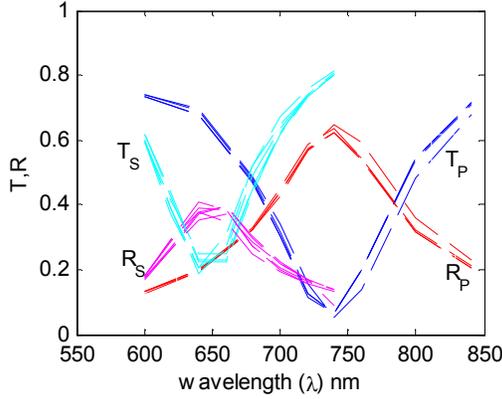
Figure 5: T and R spectra for the primary (P) and secondary (S) polarizations for various 10nm roughness iterations.
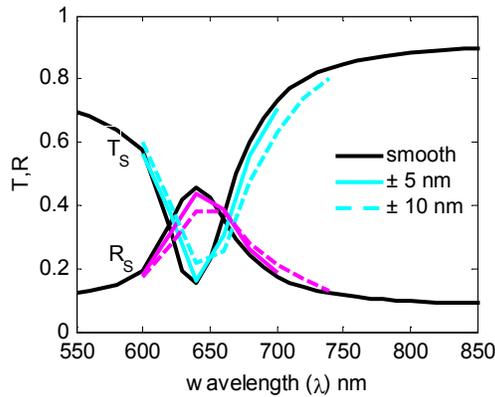
Figure 6: Spectra for the secondary (S) polarization for smooth (black), 5nm roughness (cyan), and 10nm roughness (cyan-dash).

Figure 7: Spectra for the primary (P) polarization for smooth (black), 5nm roughness (blue), and 10nm roughness (blue-dash).

Fitting the results with Lorentz curves allows us to retrieve various metrics from the spectra. These results are shown in Table 1. Here we see that the implementation of surface roughness leads to a significant shift in the primary resonance wavelength (P-peak).

Table 1: Metrics for the primary (P) and secondary (S) polarization spectra. Resonance wavelength (peak) and full-width half-max (width) in nanometers.

(nm)	Smooth	±5	±10
P-peak	720 (±3)	724 (±4)	738 (±4)
P-width	48 (±3)	52 (±5)	54 (±5)
S-peak	638 (±3)	646 (±4)	647 (±4)
S-width	35 (±3)	33 (±10)	43 (±3)

4. Conclusions

This work uses COMSOL Multiphysics to model the effects of surface roughness in nanoantenna arrays. Instead of regenerating the mesh for each roughness realization, a moving mesh is used to apply roughness, therefore preserving the DOF. Herein we see that the introduction of roughness into the nanoantenna model does not result in significant loss, but does result in a shift in the resonance wavelength. This type of result can be critical when fitting simulations to experiments, and can lead to significant error if not properly accounted for. The proposed method has much wider applications beyond nanoantennas, and even beyond electromagnetics. Most physical models make assumptions that surfaces are smooth;

however the actual roughness may have a significant effect on the simulated physical processes and therefore on the accuracy of the modeling results. This method may be applied to any model, whether mechanical, acoustic, electromagnetic, thermal, etc, in order to model the effects of roughness on the results and simulate a roughness-generated physical phenomenon.

5. References

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